**PROCEEDINGS:**

**SUPPORTING SCIENCE AND ENABLING TECHNOLOGIES FOR CLEAN LIQUID FUELS WORKSHOP**

The Supporting Science and Enabling Technologies for Clean Liquid Fuels Workshop, sponsored by the Department of Energy=s National Energy Technology Center (NETL), was held in sessions at three locations to enable wide participation:

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| San Francisco, CA | February 6, 2001 |
| Houston, TX | February 8, 2001 |
| Pittsburgh, PA | February 13, 2001 |

A total of 98 people, representing industry, academia, national laboratories, and government, participated in the three sessions.

At each location, there were breakout sessions on the following topics:

Future Fuels

Ultra-Clean Fuels

Infrastructure Reliability and Product Integrity

Petroleum Environmental Solutions

Discussion at the various sessions was lively, and many valuable comments, suggestions, and recommendations were received. These prioritized recommendations will be taken into account when preparing solicitations for this technology area.

To eliminate duplication, input from the three locations has been combined. The following includes summaries of the combined breakout presentations for all four topics, as well as a comprehensive list of all workshop participants.

## FUTURE FUELS BREAKOUT SESSION

The following fuels were identified (no priority implied):

Hydrogen

Hydrogen mixtures (AHythane@)

Methanol

Ethanol

Higher alcohols

Dimethyl ether

Other ethers

Compressed natural gas

Syngas/carbon monoxide

LPG

Oxygenates

Ammonia

Metals

Electricity

### Selected Areas of Discussion

The following topics were discussed as important for future fuels development.

Catalysts and Reactors:

- Low cost reforming technology, including load following and on-board units
- Improved models of reactor fluid dynamics
- Improved catalysts (tolerant of sulfur and higher hydrocarbons, active at milder temperatures, electrocatalysts, biomimetics, DME production)
- Improved understanding of basic chemistry and catalysis
- Air blown gasifier technology

- Direct synthesis process to bypass syngas production

Separations:

Develop:

- Processes for hydrogen separation from CO, hydrocarbon mixtures, and nitrogen
- Improved oxygen production technology, that is, processes for the separation of oxygen from nitrogen
- Improved membranes for reactors and separation processes
- Methods of Separating:
  - Separation of methanol from other compounds
  - Separation of sulfur from fuels
  - Separation of metals from heavy oils
- Process to produce syngas and simultaneously separate it from other reaction products
- Processes for carbon separation, including separation of CO from $CO_2$
- NOx traps and adsorbents to permit recycling NOx to extinction
- particulate traps
- CO tolerant fuel cells, so that CO separation won=t be necessary
- Direct methanol fuel cell

Upgrading, Blending, and Evaluation:

- De-emphasize the study of the thermodynamic properties of Fischer-Tropsch liquids
- Develop oxygenated additives for gasoline, diesel fuel, and LPG
- Evaluate AHythane@
- Study effect of contaminants in future fuels
- Develop additives to permit leak detection, particularly for hydrogen

Diagnostics and Controls:

- Develop:
  - NOx, sulfur, ammonia, hydrogen, and other sensors
  - methanol, peroxide, and calorific value detectors
  - detectors sensitive to composition changes
  - sensors/controls for multiple fuel engines (ASmart Engines@)
  - more appropriate standards and test methods and a systematic approach to specifying them

Materials:

- Materials for hydrogen storage, including materials resistant to hydrogen embrittlement
- Improved lubricants to provide superior performance with lower release of sulfur and other contaminants
- Development of fuel tolerant elastomers
- Water injection for NOx control

Systems Integration:

- Determine environmental and health effects of future fuels
- Perform life cycle cost analysis of future fuels
- Study fuel/lubricant interactions and low viscosity related wear of future fuels, including lubricants for gaseous fuels, DME, and methanol
- Study fuel system compatibility with future fuels, such as DME
- Develop fuel delivery systems for volatile fuels, such as DME, DMM, hydrogen, etc.)
- Educate the public on safety and other issues involved with future fuels
- Develop models to study the combustion chemistry and emissions of future fuels
- Develop protocols for applications testing of future fuels, including fleet testing

- Evaluate the potential for carbon sequestration relative to the integration of future fuels into the fuel use mix
- Evaluation of engineering and economic constraints of using syngas as an energy delivery system
- Study fuel production/delivery/utilization system as a whole to maximize efficiency

**Recommendations:**

- Emphasize fuels that can serve as a bridge to far-future fuels
- Develop fuel specifications
- Develop improved methods to produce hydrogen from fossil fuels
- Develop hydrogen handling and storage systems
- Focus on revolutionary, not evolutionary, concepts
- Don=t spread funding too thin
- Develop an energy strategy to help guide research
- Develop criteria for successful market penetration of future fuels (cost, customer acceptance, environmental effects, handling/fueling system, etc.)

## ULTRA-CLEAN LIQUID FUELS BREAKOUT SESSION

The Ultra-Clean Fuels discussion was targeted at the economic, environmentally friendly, and efficient use of the Nation=s fossil resources. All fuels produced must be compatible with the transportation infrastructure and formulated to enable advanced, high-efficiency engines to achieve ultra-low emissions. The following topics were identified and discussed:

- Removing significant amounts of sulfur and metals from heavy crudes.
- Developing advanced processes to economically deliver greater quantities of hydrogen.
- Converting alternative domestic resources to clean fuels that can supplement petroleum-based supplies of transportation fuels.

**Recommendations:**

High Priority

- Develop membrane technologies for syngas production, oxygen supply, etc., including developing joining technology to bond metals to ceramics.
- Develop alternatives to hydrotreating for sulfur removal
- Develop modified fuels for use in more efficient diesel engines
- Improve efficiency of gas-to-liquids production by use of advanced syngas generation, improved catalysts, and better heat management
- Evaluation of life cycle, including safety and environmental effects, of ultra-clean fuels
- Processes to produce ultra-clean fuels from domestic resources, including coal, low-quality natural gas, oil shale, etc.
- Develop economical technologies to recover hydrogen from low quality streams
- Develop improved catalysts for desulfurization, oxidative coupling, syngas conversion, and other processes, such as slurry/disposable catalysts for syngas production from coal
- Develop octane and cetane enhancers that are environmentally acceptable

- Develop technology to permit economic development of small and stranded natural gas deposits
- Focus on fundamental, rather than applications oriented, R&D
- Focus on pre-competitive technology
- Develop national energy model to evaluate the impact of refinery availability, changes in crude supply, impact of regulations, etc.

Medium Priority

- Study the chemistry of resid molecules after sulfur removal
- Develop a process that produces a clean coke
- Study coprocessing of renewables with crude
- Develop improved hydrogen generation and recovery technologies
- Develop new processing technology for resids and heavy crudes
- Develop a solid alkylation catalyst
- Perform fundamental modeling of catalysis

Low Priority

- Develop detailed hydrocarbon analysis of diesel
- Develop technology to produce clean fuels from recycled plastics and similar materials
- Develop new sulfur utilization technologies
- Study total effect on refinery of ultra-clean fuels production
- Develop process for producing liquid fuel and value added products from biomass
- Perform fundamental science to support rational harmonization of fuel quality standards

## PETROLEUM ENVIRONMENTAL SOLUTIONS BREAKOUT SESSION

This breakout group discussed needed research topics in the development of advanced technologies that will enable existing refineries to operate in an economic and environmentally sound manner and facilitate the development of new U.S.-based refinery capacity. The following technology areas were identified and discussed:

- Assessment of new risk based approaches to cleaning up existing domestic refinery sites
- Development of the next generation of advanced refinery cleanup technologies
- Identification and evaluation of means to improve permitting of new refinery units in a timely and cost effective manner
- Study and evaluation of the tradeoffs of advanced multimedia emissions (air, liquid, solid) approaches to permitting new domestic refineries
- Development of biotechnology and other novel processes to upgrade heavy and sour crude oils for refining in existing refineries

**Recommendations:**

High Priority

- Perform life cycle analysis of bio-upgrading of crude
- Study metals and catalyst recovery to get a better understanding of metals in the refinery
- Develop technology for $CO_2$ separation and utilization
- Develop new uses for petroleum coke
- Develop technology to efficiently and reliably produce syngas from refinery wastes
- Develop novel processes to upgrade heavy and sour crudes
- Improve distillation and develop other separation processes, including hybrid processes
- Study permitting issues and how permit changes at one unit affect other units

- Develop alternative processing technologies that would be more environmentally benign, that is, less energy intensive and with fewer waste products
- Develop and standardize analytical techniques for heavy fractions, including sulfur analysis
- Develop new hydrocracking catalysts, e.g., nanosize
- Develop advanced analytical technologies for pollution control and catalyst characterization
- Develop biotechnology and other novel processes for heavy/sour crudes
- Develop basic science to allow expediting of permitting
- Develop next generation of advanced refinery cleanup technology

Medium Priority

- Develop new and improved wastewater/sludge/oil treating systems
- Reduce the cost and improve the reliability of monitoring to allow feed forward control.
- Develop biotechnology to desulfurize crudes
- Develop techniques to recover metals from used catalysts
- Develop processes for upgrading waste products
- Study optimization of processing between production site and refinery
- Improve integration of heat and power management in refineries

Low Priority

- Develop soil remediation technologies
- Improve contaminant plume modeling
- Improve NOx, PM, $SO_2$, etc. monitoring and control
- Study the effect of MTBE in groundwater and the effect of MTBE substitutes on the environment
- Develop technology to monitor and control greenhouse gas emissions

- Develop novel technologies for better utilization of by-product streams
- Address needs of independent refiners

## INFRASTRUCTURE RELIABILITY AND PRODUCT INTEGRITY BREAKOUT SESSION

This breakout group discussed needed research topics in the development of advanced technologies that enable:

- In-situ monitoring of petroleum pipelines, tanks, and transfer points
- New methods of product handling and segregation to prevent contamination as the number of fuel specifications increases
- On-line analysis and analytical measurement tools to ensure proper product distribution
- Advanced diagnostics and risk assessment technologies focused on preventing releases into the air, water, and ground

**Recommendations:**

High Priority

- Develop a better national model of the entire fuels distribution system
- Perform overall system cost/benefit analysis of boutique fuels, and eliminate some boutique fuels, replacing them with a smaller number of fuels with better environmental properties
- Look at optimized new fuel/engine systems to improve emissions and efficiency
- Develop method for detection of third party damage to pipelines
- Develop remote leak detection and remediation capability
- Assure integrity of product delivery through control and measurement strategies
- Harmonize standards for liquid pipelines
- Develop techniques to permit laboratory studies of the effect of future fuel candidates on the transportation and storage infrastructure
- Develop real-time, in-situ analytical techniques for sulfur and other fuel properties

- Develop cost-effective pipeline cleaning technology
- Develop techniques for sulfur removal at the terminal

Medium Priority

- Develop analytical technique for determining low levels of sulfur in real time
- Evaluate infrastructure needs for refineries producing ultra-clean fuels
- Develop understanding of adsorption/desorption phenomena in pipelines, mixing at interfaces, and develop methods to clean pipelines
- Develop additives or technology to alleviate problems associated with introduction of ultra-clean fuels
- Study blending, compatibility, and storage stability of future fuels
- Study interactions of all aspects of the refinery/pipeline infrastructure and model the infrastructure=s vulnerabilities

Low Priority

- Look at alternatives to pipelines (barges, railroads, trucks)
- Develop nondestructive techniques for determining pipeline integrity
- Develop improved techniques for cleanup after pipeline spills
- Develop better and cheaper interface detectors
- Develop ways to make flow in pipelines more plug-like
- Develop and adopt new standardized ASTM methods, including round robin testing of new methods